MSTe NEWS

August 2018
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INSIDE

Los Alamos NATIONAL LABORATORY EST.1943

As a member of Nuclear Materials Science (MST-16) DeeAnn Chavez coordinates complex projects supporting the Lab's mission.
Photo by Shannan Winchell, XIT-TSS

DeeAnn Chavez

Taking care of business from start to finish

By H. Kris Fronzak, ADEPS Communications

DeeAnn Chavez hangs up the phone, looking satisfied. She's putting the last touches on a complicated project that's been years in the making: disposing of 10 years' worth of accumulated legacy waste—mainly plutonium and uranium—for Nuclear Materials Science (MST-16) at Los Alamos National Laboratory.

"... I work with amazing people who take pride in their work, do whatever it takes to get the job done, and strive to meet the Lab's mission. I am honored to be part of this group."

"MST-16 is the end of the line in terms of materials processing and we were approaching maximum capacity, which made this a really important project for the Laboratory," Chavez said. "I'm working with program management to add ongoing legacy disposal to our budgets going forward and making sure we have procedures in place to regularly manage waste."

This is one of several complicated projects that Chavez coordinates from beginning to end as one of the group's technical project managers.

continued on page 3

From David's desk . . .

As summer is ending and MST is updating our five-year staffing planning exercise, I've been examining how our division has grown over the last couple of years and is improving our overall diversity. Over the last two years, MST Division's budget has grown from $74M to $85M and our workforce has grown from 126 to 150 regular staff members while losing 17 people due to retirements and other attrition. This growth has occurred primarily in the nuclear weapons programs, but also in our science and applied energy programs. In the five-year projections, we envision increasing our budget in these same program areas to about $97M (+$12M over FY18) and increasing our workforce to about 175 regular, full-time employees. As shown in the tables below, we have been improving the diversity of our workforce but still have significant progress to make. Perhaps most striking in this staffing analysis was that our average age has significantly decreased from 46.4 to 43.8 years of age. The fact that we have a younger workforce emphasizes the need for a strong mentoring program.

MST has begun a mentoring program for our new hires and hopefully you have all met with your group leaders to identify possible mentors for you. To improve the student experience, PADSTE has revamped the mentor training to better prepare our student mentors. I would like to point out that we all have a role in mentoring each other. Just as it takes a village to raise a child, it also requires a community of mentors to educate a student or new hire. We rely on the mentors for setting the expectations for our safety, security, and science culture. Additionally, we rely on other co-workers (scientists, technologists, and technicians) in MST to train our new workers. Therefore, my expectation is that all workers are helping to instill a strong safety, security, and science culture in MST.

> *"I would like to point out that we all have a role in mentoring each other. Just as it takes a village to raise a child, it also requires a community of mentors to educate a student or new hire."*

With this growth in employees we are feeling a space stress, especially in the TA-35/55 corridor. For ADEPS/PADSTE I am leading a strategic space analysis in the Pajarito Corridor, which is creating the business case for increased office and lab space needs in that area. As a first step, we have made the case for taking over the old TRIDENT building, primarily to establish a nuclear fuel fabrication capability but also to integrate some of our polymer additive manufacturing with AET Division. With the TRIDENT building acquisition,

continued on next page

Job Class	Regular Full-time Staff			Pipeline	
	R&D Scientist/Engineers	Technician/ Technologists	Overall	Postdocs	Students
2016	19%	21%	26%	23%	34%
2017	21%	18%	26%	22%	33%
2018	24%	16%	26%	31%	35%

Percentage of female employees per job class and pipeline.

Job Class	Regular Full-time Staff			Pipeline	
	R&D Scientist/Engineers	Technician/ Technologists	Overall	Postdocs	Students
2016	7%	67%	30%	5%	24%
2017	13%	62%	32%	13%	26%
2018	11%	54%	31%	15%	31%

Percentage of under-represented minority employees (African-American, Hispanic/Latino, and Native American) per job class and pipeline.

From David's desk cont.

we will gain significant unclassified office space. In planning for a future facility, MST has partnered with Sigma, MPA, AET, and PT divisions to submit a proposal to NNSA for a new Advanced Manufacturing Science Center (a 70,000-sq.-ft. facility) that includes classified and unclassified offices and laboratory space.

Lastly as the summer is ending, we may have a number of distractions—vacations, students returning to school, contract transition, etc. Please help each other stay focused on performing our work safely. For mentors or PICs that may be leaving town, ensure that we assign alternate mentors and PICs so that we have appropriate oversight in our work areas.

We look forward to seeing you at the MST Division picnic. Have a great rest of your summer!

MST Division Leader David Teter

Chavez cont.

"It would be difficult to keep the group running successfully without DeeAnn's oversight," said MST-16 Group Leader David Pugmire. "She's an integral part of the group management."

The legacy waste project Chavez is wrapping up resulted from years of planning and execution. Her role was to manage the removal of the waste—securing funding, supporting technicians as they identified and organized samples, collaborating with other program managers, and overseeing sample oxidization and eventual disposal. In total, her team safely removed 1.6 kilograms' worth of small samples from PF-4, the Lab's central plutonium facility.

"This was a big project, but DeeAnn is great at picking up on what needs to be done and making it happen," Pugmire said.

Being highly organized is second nature to Chavez, an Española native who grew up watching her father plan the welding and mechanical projects he undertook as side jobs. Inspired by his methodical, detail-oriented approach, Chavez studied business administration at the University of New Mexico and joined the Lab in 2006 as an undergraduate student supporting quality assurance.

A keen interest in weapons research and in maintaining the nation's nuclear stockpile led Chavez to join MST-16. The group is responsible for characterizing new and aged plutonium pit materials, investigating actinide materials, and developing analysis technologies. This broad scope of work makes her job varied and sometimes hectic. On any day, her role might involve planning for projects, overseeing the group's budget, or procuring funds for classified projects.

Chavez's attention to detail earned her a Distinguished Performance Award in 2011 as part of the U.S. Special Project Team. For more details on this accomplishment see her "favorite project" described at right.

Her next big project? Spearheading modernization of MST-16's numerous gloveboxes. Los Alamos is the nation's Plutonium R&D Center of Excellence, tasked with producing 30 plutonium pits every year. Recently, the U.S. government asked the Lab to expand pit production abilities with a "surge" capability. MST-16 is rising to that challenge by updating its existing gloveboxes to process plutonium, and Chavez is managing this glovebox project in key ways: helping techs dispose of radioactive equipment, procuring new tools, and juggling logistics.

"Operations is where the rubber meets the road. It takes a lot of coordination and effort to get work done, especially at TA-55. Fortunately, I work with amazing people who take pride in their work, do whatever it takes to get the job done, and strive to meet the Lab's mission," she said. "I am honored to be part of this group."

DeeAnn Chavez's favorite project

In 2011, I received a Distinguished Performance Award as part of the U.S. Special Project Team. As the lead quality representative for a project involving the United Kingdom's Ministry of Defense, I was responsible for ensuring DOE and customer requirements were satisfied while manufacturing materials.

The team combined technical, management, and administrative personnel to overcome challenges that required innovative thinking and creativity by each team member. The end result was successfully meeting our British customer requirements and specifications.

From the project's inception, we had to improvise and be flexible in order to meet deliverables on time. Each hurdle required a unique approach, demonstrating the team's dedication to its motto: "work through the issues and find solutions."

This work opened many doors for future collaborations, demonstrating that cultural differences do not impede any task or accomplishment.

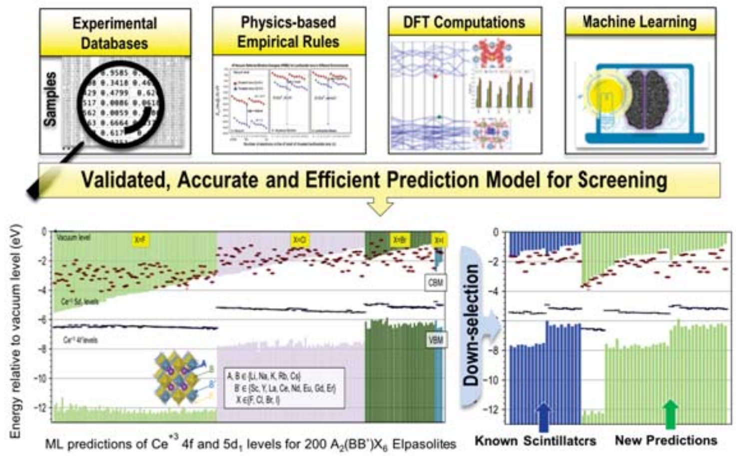
Physics-informed machine-learning model may streamline performance of inorganic scintillators

Using past experimental data, Materials Science and Technology Division researchers trained a machine-learning model to predict a key aspect of scintillator performance instantly and with high accuracy. Their approach overcomes the traditional lengthy and challenging first-principles route for such a prediction crucial to optimizing electronic structure of inorganic scintillators. The advance enables high-throughput explorations of vast chemical spaces to promote the discovery of inorganic scintillators.

Applications of inorganic scintillators—activated with lanthanide dopants, such as cerium—are found in diverse fields. As a strict requirement to exhibit scintillation, the 4*f* ground state and 5d_1 lowest excited state levels induced by the activator must lie within the host bandgap. The team's machine learning–based screening strategy builds on well-known, physics-based chemical trends for the host-dependent electron-binding energies within the lanthanide activator's 4*f* and 5d_1 energy levels and available experimental data. It uses high-throughput prediction of the lanthanide dopants' ground and excited state energy levels to rapidly, reliably estimate the relative positions of the activator's energy levels relative to the valence and conduction band edges of any given host chemistry.

The model's predictions were validated by a comparison with past experimental data on perovskites. This comparison showed that the developed approach can both capture systematic chemical trends across host chemistries and therefore effectively screen promising compounds in a high-throughput manner—as demonstrated by applying the model on 200 elpasolite compounds.

While a number of other application-specific performance requirements need to be considered for a viable scintillator, the present scheme can be a practical tool to systematically down-select the most promising candidate materials in initial screening for a subsequent in-depth investigation. The team has made two LANL innovation disclosures based on the findings of this work.



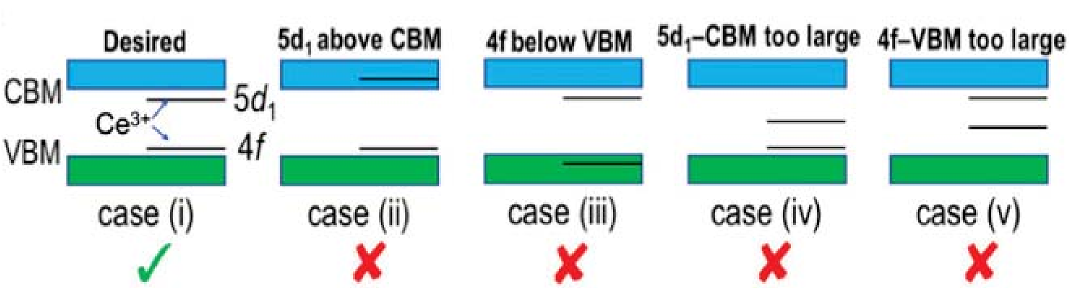
Different key components of the newly developed approach that jointly provide high-throughput predictions of lanthanide activator levels in a given host chemistry for a first-line screening of viable scintillator chemistries.

This work, which relied on the Lab's high-performance computing resources, was funded by Los Alamos's Laboratory Directed Research and Development program. It supports the Laboratory's Energy Security mission and Materials for the Future science pillar, including its emergent phenomena science theme. Los Alamos pursues the science and engineering needed to establish design principles, synthesis pathways, and manufacturing processes that advance and create materials with controlled functionality and predictive performance to solve national security science challenges.

Researchers: Ghanshyam Pilania, Kenneth McClellan, Chris Stanek, and Blas Uberuaga (Materials Science in Radiation and Dynamics Extremes, MST-8).

Reference: *Journal of Chemical Physics* **148**, 241729 (2018).

Technical contact: Ghanshyam Pilania



A schematic illustration comparing ideal [case (i)] versus non-ideal [cases (ii-v)] placements of the Ce^{3+} 4*f* and 5d_1 levels in a host material from a scintillation performance point of view.

All-solid-state cryocooler becomes a reality

The ability to cool objects to cryogenic temperatures transcends many disciplines and is essential to a wide range of scientific and national security applications. To date, mechanical refrigeration has been the only technology for cryocooling devices that operate continuously in remote locations such as in space. However, all mechanical cryocoolers have moving parts that not only limit their reliability but also introduce mechanical vibrations and microphonic noise that limit system performance. Markus Hehlen (Engineered Materials, MST-7) and collaborators have—for the first time—demonstrated an all-solid-state optical refrigerator that operates at cryogenic temperatures and has no moving parts. Their work represents a breakthrough in cryogenics. It has been published in the *Nature* journal *Light: Science & Applications* and was featured in *Nature Photonics*.

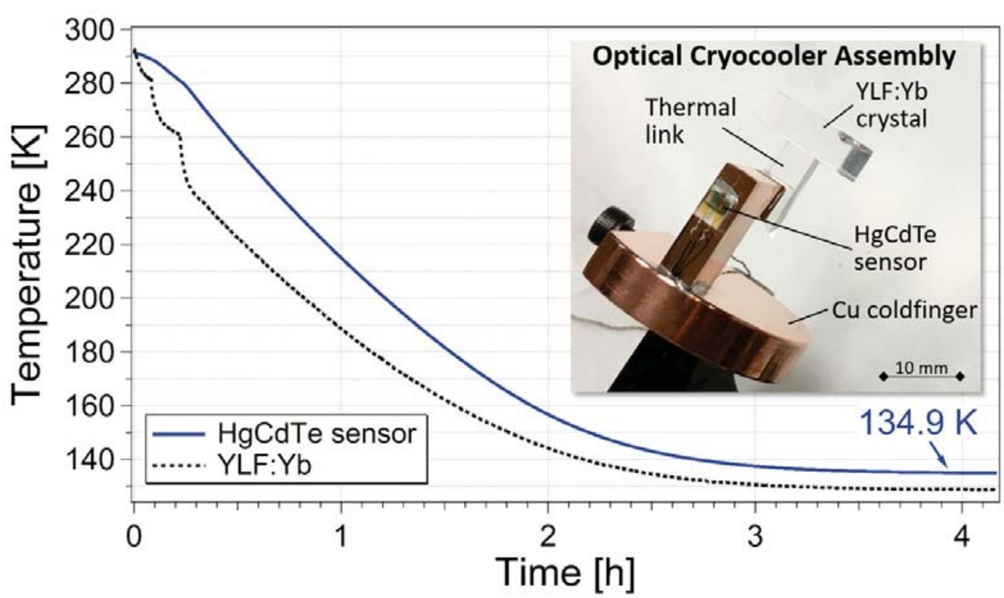
All-solid-state cryocooling is an optical effect that occurs in certain materials via anti-Stokes fluorescence. In this process, a solid is excited by a laser and subsequently fluoresces at a slightly greater mean energy (shorter wavelength) than that of the exciting laser. The corresponding energy difference is provided by phonon energy (heat) that is extracted from the solid and carried away as light, thus cooling the solid in the process. This effect was first observed by Richard Epstein at Los Alamos National Laboratory in 1995. Ultrapure rare-earth-doped crystals such as Yb^{3+}-doped $YLiF_4$ (YLF:Yb) developed by the project team over the past two decades are particularly suited as they offer the required spectrally narrow optical transitions and >99% quantum yields.

Previous work had only cooled the YLF:Yb crystal itself. Cooling a useful payload such as a sensor by using a YLF:Yb crystal, however, posed a range of additional engineering challenges. In the most recent effort, the team developed (1) a custom-shaped thermal link that connected the YLF:Yb crystal to the sensor with good thermal conductivity while rejecting the intense crystal fluorescence, (2) an adhesives-free bond between the thermal link and the YLF:Yb crystal, and (3) silica aerogel supports that secured the cooled assembly inside the cryocooler with minimal conductive heat load. These advances have enabled laser-cooling of a HgCdTe infrared sensor to 135 K for the first time (see figure). This represents a breakthrough in the field of cryogenics and opens the door to using this technology for a variety of applications that benefit from a reliable cryogenic refrigerator having no moving parts and no associated vibrations.

The project team was led by Hehlen (MST-7) and included Christopher Hamilton (MST-7), Steven Love (Space and Remote Sensing, ISR-2), Kevin Baldwin (Center for Integrated Nanotechnologies, MPA-CINT), Tana Cardenas (MST-7), Todd Williamson (Nuclear and Radiochemistry, C-NR), and University of New Mexico collaborators Junwei Meng, Alexander Albrecht, Eric Lee, Aram Gragossian, Richard Epstein, and Mansoor Sheik-Bahae.

This research supports the Laboratory's Science of Signature mission and Materials for the Future science pillar. The work leverages Los Alamos's expertise in high-purity inorganic synthesis, halide crystal growth, thin-film deposition, silica aerogel fabrication, optical spectroscopy, high-power lasers, and thermal/optical system design. The work used Lab capabilities such as the Target Fabrication Facility, the Center for Integrated Nanotechnologies, and the TA-46 cleanroom infrastructure to realize the first optical cryocooler prototype.

Technical contact: Markus Hehlen



Solid-state laser cooling of a HgCdTe sensor to 135 K using a YLF:Yb crystal. The solid curve shows the sensor temperature as a function of time after turning on the pump laser (47 W at 1020 nm). The inset is a picture of the optical cryocooler assembly developed in this project.

MST fosters research opportunities with second university outreach workshop

Event featured research from across the Lab, more than a dozen university presentations

Materials Science and Technology Division hosted its second University Outreach Workshop at Los Alamos National Laboratory on August 1-2. The workshop, held in the Materials Science Laboratory, focused on recent research, novel techniques, and unique capabilities in manufacturing science. Presentation topics included studying materials with additive manufacturing, applying techniques to understand material failure, and industrializing metal powder bed fusion.

The event featured a mix of talks by university professors and Los Alamos researchers and two poster sessions geared to highlight research done at the Lab. The aims of this two-day workshop were to identify talent to strengthen the next-generation workforce, establish student exchange opportunities, accelerate the development of technology, and help young Lab scientists establish a network of collaborators.

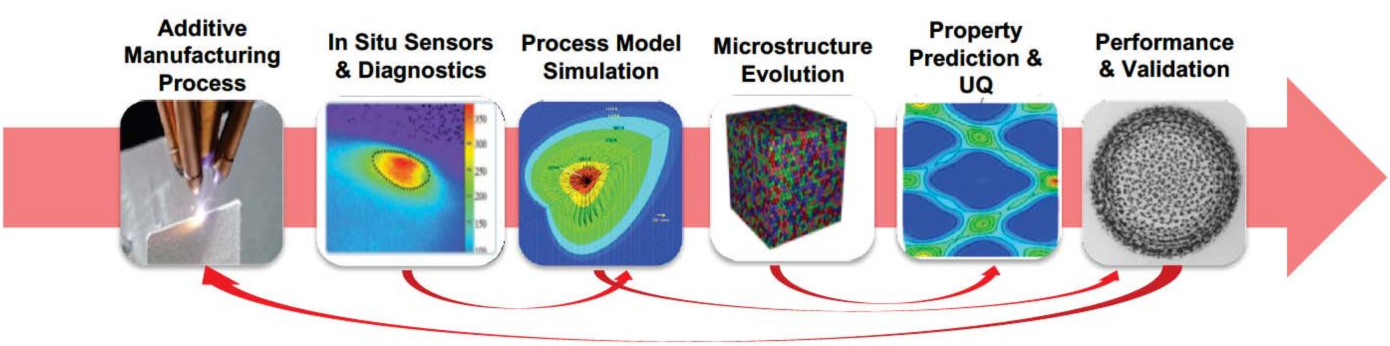
This year's workshop was organized by Kim Obrey and Laurent Capolungo (Materials Science in Radiation and Dynamics Extremes, MST-8), Clarissa Yablinsky (Nuclear Materials Science, MST-16), Brian Patterson (Engineered Materials, MST-7), and John Carpenter (Finishing Manufacturing Science, Sigma-2).

The workshop was funded by the Momentum Initiative, which is owned by the Associate Directorate for Experimental Physical Sciences. The program sponsors the engagement of scientific communities to enhance Laboratory strategic partnerships, especially in the arena of mesoscale science.

MST's inaugural university workshop, dedicated to nuclear materials, involved more than 10 organizations and prompted new university collaborations and two joint proposals funded by the Department of Energy: an Energy Frontier Research Center called FUTURE (for Fundamental Understanding of Transport Under Reactor Extremes) and a second nuclear energy research proposal funded through the Nuclear Energy University Program.

Laboratory researchers use an extruder in the Lab's Sigma Complex to perform manufacturing research essential to the Lab's mission.

Technical contact: Laurent Capolungo



Manufacturing science can be defined as the application of fundamental science research and development activities in order to understand the critical steps in the manufacturing process for the purposes of control and optimization. To learn more about manufacturing science, an area of materials science leadership at Los Alamos National Laboratory, please see www.lanl.gov/science-innovation/_assets/docs/manufacturing-science.pdf.

Prism chair Roberta Beal (pictured here with Prism co-chair Mike Davis at the Out in Science, Technology, Engineering, and Mathematics conference) helped bring an LGBTQ+ pride event to Los Alamos.

Diversity snapshot: strong across eight types of jobs

The Laboratory's workforce is much richer with diversity than the Department of Energy labs overall—40 % of Los Alamos employees are described as "underrepresented minorities" compared to the national lab average of 17 %.

Hispanics and Latinos have the biggest presence at the Laboratory, followed by Native Americans and African Americans.

From undergraduate students to senior leadership, LANL's diverse demographics are stronger across all eight types of jobs covered in the most recent statistics (from 2017), which the Lab posts publicly (see www.lanl.gov/careers/diversity-inclusion/index.php).

Lab's LGBTQ+ group participates in first Los Alamos Pride

For the first time, members of the Los Alamos community came together to celebrate LGBTQ+ pride on home turf on June 15 at Fuller Lodge.

Prism, the Lab's Lesbian, Gay, Bisexual, Transgender, and Queer+ (LGBTQ+) Employee Resource Group (ERG), staffed a booth and participated in the activities on behalf of the Laboratory. Prism fosters an inclusive workplace culture, promotes visibility, and strives to maintain diversity across the Lab through events and networking.

The community festival included educational information from local LGBTQ+ organizations and activities that ranged from karaoke to lawn games.

HeadsUP!

Materials Science Complex heeds the call to "bring out your dead" vacuum pump

By leveraging an existing project to optimize lab space in the Materials Science Laboratory (MSL), MST staff and members of the Environmental Protection and Compliance (EPC) and Condensed Matter and Magnet Science (MPA-CMMS) organizations have successfully recycled 44 vacuum pumps.

This project is an example of the Lab meeting its institutional environmental objectives to clean the past by continuing to dispose of equipment no longer in use. It also provided a cost-effective method of managing the recycle of the old vacuum pumps in a large group instead of managing them a few at a time.

In FY18, MST Division received funding to improve lab space in the Materials Science Laboratory. In cleaning out two labs, staff located four vacuum pumps to drain and recycle. To take advantage of this effort, they then put out the call to the entire Materials Science Complex to collect more vacuum pumps.

Nuclear Materials Technology (MST-16) staff working in the MSL agreed to help drain the pumps and pack them with vermiculite. Materials Physics and Applications management approved MST-16 staff to work under its existing integrated work processes. Staff from deployed Environment, Safety, and Health Facilities (STO-FOD) ensured requirements for safely draining the oil, testing, and proper disposal were met.

Participants included Iven Gonzales, Mark Ortega, Chris Baxter, and Carlos Archuleta (MST-16); Patricia Vardaro-Charles (Waste Management Programs, EPC-WMP); Mike Hundley (MPA-CMMS); and Chris Serazio (Waste Management Services, EPC-WMS).

Celebrating service

Congratulations to the following MST Division employees celebrating recent service anniversaries:

Joseph Martz, MST-DO .... 35 years
Terry Holesinger, MST-16 .... 25 years
Kenneth Mcclellan, MST-8........ 25 years
Bryan Bennett, MST-7 .... 20 years
Richard Salazar MST-16 .... 20 years
Dominic Peterson, MST-7........ 15 years
Tarik Saleh, MST-8 .... 15 years
Zachary Smith, MST-7........ 10 years
John Lamar, MST-7 .... 5 years
Ghanshyam Pilania, MST-8........ 5 years
Reeju Pokharel, MST-8 .... 5 years
Miranda Williams MST-16 .... 5 years

MST e NEWS

Published by the Experimental Physical Sciences Directorate.

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NNSA National Nuclear Security Administration